

Theory for the reduction of products of spin operators

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Abstract

In this study we show that the sum of the powers of arbitrary products of quantum spin operators such as $(S^+)^l(S^-)^m(S^z)^n$ can be reduced by one unit, if this sum is equal to $2S + 1$, S being the spin quantum number. We emphasize that by a repeated application of this procedure *all* arbitrary spin operator products with a sum of powers larger than $2S$ can be replaced by a combination of spin operators with a maximum sum of powers not larger than $2S$. This transformation is exact. All spin operators must belong to the same lattice site. By use of this procedure the consideration of single-ion anisotropies and the investigation of the magnetic reorientation within a Green’s function theory are facilitated. Furthermore, it may be useful for the study of time dependent magnetic properties within the ultrashort (fsec) time domain.

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A renewed interest in the properties of spin operators and their products is caused by the investigation of the magnetic anisotropy and other magnetic properties of thin films and multilayers [1]. In general the lattice anisotropies are defined by the expansion of the free

energy $F(T, \Theta, \Phi)$ in powers of the direction cosines, or by a complete set of spherical harmonics $Y_{lm}(\Theta, \Phi)$ [2], with Θ and Φ being the polar and the azimuthal angles, respectively. The coefficients of this expansion are temperature dependent, these *effective* anisotropy coefficients are measurable quantities [3,4]. To compare the measurements with first principle electronic calculations of the *microscopic* anisotropy parameters at $T = 0$ [5,6], the temperature dependences of the effective anisotropies have to be known [7–9].

The magnetic lattice anisotropy is mainly a single-ion property. Corresponding to the atomic lattice symmetry, they can be represented in the Hamiltonian by powers of the components of the three-dimensional Heisenberg spin S^α , $\alpha = x, y, z$, and mixed products of these spin operators. By use of this generalized Heisenberg-type Hamiltonian the magnetic properties, in particular the effective anisotropies, can be determined by the usual rules of Statistical Mechanics [7,8,10,11]. Note that in addition to the *diagonal* operators such as $(S^z)^n$ or $(S^- S^+)^n$, also *non-diagonal* operators may occur. Here we have introduced the non-hermitean raising and lowering spin operators $S^\pm = S^x \pm i S^y$, assuming the quantization axis along the z -direction. This direction may be the easy axis of the magnetization determined by the anisotropies, for example. Due to an external magnetic field the spins are tilted away from the easy axis. Then by application of the usual rotation properties of spin operators [12], non-diagonal spin operators are introduced in the Hamiltonian.

For a single-spin problem, the respective expectation values of spin operators can be easily deduced from simple diagonalization [8,10,11]. However, in the case of interacting extended systems, in which the magnetic moments are coupled by the exchange interaction, approximations are necessary. The exchange coupling is in general much stronger than the involved anisotropies. Within a mean field approximation the system is reduced to an effective single-particle system, subject to a molecular field due to the exchange coupling [8,10,11]. This approach yields a bad description of the magnetization in particular for low-dimensional systems, since collective excitations (spin-waves) of the Heisenberg magnet are neglected. These spin fluctuations are considered by spin-wave theories. For instance, the Holstein-Primakoff approach has been applied frequently [13,14], which is valid for low tem-

peratures. On the other hand, the Green's function method [15–17] and the Schwinger-Boson approximations [18,19] can be used also at higher temperatures, since they consider partly interactions between spin-waves. The Green's function method is a hierachical approach, i.e. in the respective equation of motion appear higher order Green's functions consisting of a larger number of spin operators [15,16]. In order to obtain a closed set of equations for the Green's functions, the higher order ones have to be decoupled, i.e. approximated by lower order ones at a certain level of hierarchy.

The single-ion lattice anisotropies are taken into account by *local* Green's functions, i.e. consisting only spin operators of a single lattice site. Such local Green's functions with non-diagonal operators appear within the spin wave treatment of the magnetic reorientation [17], or in the case of a noncollinear magnetism. In this study we will show that under certain conditions the higher order local Green's functions appearing in the equation of motion, or the respective expectation values as obtained from the spectral theorem, can be replaced by lower order ones. This will be the case for general products of spin operators such as $(S^x)^l(S^y)^m(S^z)^n$ or $(S^+)^l(S^-)^m(S^z)^n$, if the sum of their powers (the 'total power') is $l+m+n = 2S+1$, S being the (integer or half-integer) spin quantum number. In this case the total power can be reduced by one unit, resulting then in lower order Green's functions or expectation values. Any combination of spin operators can be reduced, in particular also non-diagonal ones such as $(S^\pm)^m(S^z)^{2S+1-m}$. This procedure is exact. The reason for this property is the fixed magnitude of the spin operator \mathbf{S} , i.e. $(\mathbf{S})^2 = (S^x)^2 + (S^y)^2 + (S^z)^2 = S(S+1)$, thus the three components are not independent of each other. Furthermore, by a repeated application of this procedure also spin operator products with a sum of powers larger than $2S+1$ can be reduced correspondingly to a total power equal to $2S$. We are not aware in the literature about such a reduction in general. The outlined procedure seems to be a special case of the relationships between irreducible unit tensor operators with different rank [12,20]. In a forthcoming paper we will investigate this connection into greater detail.

Quantum mechanical spins are characterized by the commutation relations $[S^+, S^-] = 2S^z$ and $[S^z, S^\pm] = \pm S^\pm$, in units of $\hbar \equiv 1$. As mentioned, the spin operators under

consideration belong to the same Heisenberg spin \mathbf{S} , thus a particular lattice site index is omitted here. In case of time dependent spin operators the same time for all operators is assumed. The description of the reduction of the spin operator products is performed within several steps. As an example we show the respective procedure of the particular product $(S^-)^m (S^z)^{2S+1-m}$. Other combinations can be obtained similarly, or by application of the commutation relations between spin operators.

1) First we state the general property for the raising and lowering operators,

$$(S^-)^{2S+1} = (S^+)^{2S+1} = 0. \quad (1)$$

2) From the the general identity [15,16]

$$\prod_{i=-S}^S (S^z - i) = 0, \quad (2)$$

one can deduce the first reduction in the total power of spin operator products, namely

$$(S^z)^{2S+1} = \sum_{i=0}^{2S} \alpha_i^{(S)} (S^z)^i, \quad (3)$$

the $\alpha_i^{(S)}$ being rational coefficients dependent on S , which can be determined for each S with the help of a recursion relation from coefficients of lower S . In particular one obtains

$$\begin{aligned} \text{integer } S : \quad (S^z)^{2S+1} &= S^z \sum_{i=0}^{S-1} \alpha_{2i}^{(S)} (S^z)^{2i}, \\ \text{half - integer } S : \quad (S^z)^{2S+1} &= \sum_{i=0}^{S-1/2} \alpha_{2i}^{(S)} (S^z)^{2i}. \end{aligned} \quad (4)$$

The coefficients $\alpha_i^{(S)}$ for the minimal and the maximal index i can be given in closed form,

$$\begin{aligned} \text{integer } S : \quad \alpha_0^S &= -S^2 \alpha_0^{(S-1)} = (-1)^{S-1} \prod_{i=0}^{S-1} (S-i)^2, \\ \alpha_{2S-2}^S &= \alpha_{2S-4}^{(S-1)} + S^2 = \sum_{i=0}^S i^2; \\ \text{half - integer } S : \quad \alpha_0^S &= -S^2 \alpha_0^{(S-1)} = (-1)^{S-1/2} \prod_{i=0}^{S-1/2} (S-i)^2, \\ \alpha_{2S-1}^S &= \alpha_{2S-3}^{(S-1)} + S^2 = \sum_{i=0}^{S-1/2} \left(i + \frac{1}{2}\right)^2. \end{aligned} \quad (5)$$

For the other indices the recursion relations are given by

$$\alpha_{2i}^S = \alpha_{2i-2}^{S-1} - S^2 \alpha_{2i}^{S-1}, \quad (6)$$

with $2i = 2, \dots, 2S - 4$ for integer S , and $2i = 2, \dots, 2S - 3$ for half-integer S .

3) Consider now the general spin identity

$$(S^z)^2 = S(S+1) - S^z - S^- S^+. \quad (7)$$

For the determination of the products $(S^-)^m (S^z)^{2S+1-m}$ multiply Eq.(7) *from the right* subsequently by $(S^z)^l$, $l = 2S - 1, \dots, 1$. Calculate at first for $l = 2S - 1$ with the help of Eq.(3) the product

$$(S^z)^{2S} = \sum_{i=0}^{2S-1} \beta_i^{(S,2S-1)} (S^z)^i - S^- S^+ (S^z)^{2S-1}, \quad (8)$$

the coefficients $\beta_i^{(S,2S-1)}$ depend on the $\alpha_i^{(S)}$ and have to be determined for each S . Calculate then subsequently for $l = 2S - 2, 2S - 3, \dots, 1$ the products

$$(S^z)^{l+1} = \sum_{i=0}^l \beta_i^{(S,l)} (S^z)^i + S^- S^+ \sum_{i=l}^{2S-1} \gamma_i^{(S,l)} (S^z)^i, \quad (9)$$

with corresponding coefficients $\beta_i^{(S,l)}$ and $\gamma_i^{(S,l)}$ dependent on S , with $\gamma_{2S-1}^{(S,2S-1)} = -1$. Within this procedure the product $(S^z)^{l+2}$ appearing for each value of l has to be replaced by the result of the preceding calculation for $l + 1$. Finally, for $l = 0$ one obtains an expression for S^z given by

$$S^z = \beta_0^{(S,0)} + S^- S^+ \sum_{i=0}^{2S-1} \gamma_i^{(S,0)} (S^z)^i. \quad (10)$$

Eqs.(3), (8), (9), and (10) form a set of equations for the powers of S^z ranging from 0 to $2S + 1$. The products $S^- S^+ (S^z)^i$ remain unchanged at present. These equations can be viewed to represent relations between spin operators as well as between the respective expectation values.

4) By application of Eqs.(8) – (10) we are now in the situation to reduce the sum of powers of the spin operator products $(S^-)^m (S^z)^{2S+1-m}$ by one unit. Consider at first the product

$(S^-)^{2S} S^z$ ($m = 2S$), and replace the operator S^z by Eq.(10). Due to $(S^-)^{2S+1} = 0$, Eq.(1), the terms consisting $S^- S^+$ on the right hand side of Eq.(10) vanish, yielding

$$(S^-)^{2S} S^z = \delta_0^{(S,2S)} (S^-)^{2S} = \beta_0^{(S,0)} (S^-)^{2S} = S (S^-)^{2S}. \quad (11)$$

The latter identity is obtained from inspection. The total power of the product $(S^-)^{2S} S^z$ has thus reduced by one unit.

5) Consider now subsequently the products $(S^-)^m (S^z)^{2S+1-m}$ with $m = 2S-1, \dots, 1$. As in the preceding step, replace the operator $(S^z)^{2S+1-m}$ with the help of Eq.(9) for $l+1 = 2S+1-m$. Use then the result for the preceding spin operator product $(S^-)^{m'} (S^z)^{2S+1-m'}$ with $m' = m+1$. Within the course of these calculations one has to commute the product $S^+ (S^z)^i$ by use of $S^+ (S^z)^i = (S^z - 1)^i S^+$, replace the product $S^- S^+$ by the identity Eq.(7), and finally solve the result for $(S^-)^m (S^z)^{2S+1-m}$. Together with Eqs.(3),(11) a set of equations is obtained for the products

$$(S^-)^m (S^z)^{2S+1-m} = (S^-)^m \sum_{i=0}^{2S-m} \delta_i^{(S,m)} (S^z)^i, \quad (12)$$

for $0 \leq m \leq 2S$. As can be seen, the products of the left hand side of Eq.(12), with the total power equal to $2S+1$, have been replaced by a sum of spin operator products whose maximal sum of powers is $2S$. Thus the total powers of the original spin operator products have been reduced by one unit. The rational coefficients $\delta_i^{(S,m)}$ depend on the spin quantum number S . For $m = 0$ they are given by the coefficients $\alpha_i^{(2S)}$ of Eq.(3). In Table 1 we present results for $\delta_i^{(S,m)}$ for several values of the spin quantum number S . For the maximal index $i = 2S-m$ one obtains from inspection $\delta_{2S-m}^{(S,m)} = m(2S+1-m)/2$, furthermore for integer S one has $\delta_0^{(S,1)} = 0$. As an example for the reduction procedure and for the use of the Table 1 we show explicitly the respective results for the case $S = 2$. The products of spin operators $(S^-)^m (S^z)^{2S+1-m}$ with a total power of $2S+1 = 5$ is replaced by a series with increasing powers of S^z , and a maximum total power of $2S = 4$.

$$(S^z)^5 = -4 S^z + 5 (S^z)^3$$

$$S^- (S^z)^4 = -2 S^- S^z + S^- (S^z)^2 + 2 S^- (S^z)^3$$

$$(S^-)^2 (S^z)^3 = -2 (S^-)^2 S^z + 3 (S^-)^2 (S^z)^2$$

$$(S^-)^3 (S^z)^2 = -2 (S^-)^3 + 3 (S^-)^3 S^z$$

$$(S^-)^4 S^z = 2 (S^-)^4$$

$$(S^-)^5 = 0$$

6) To consider the spin operator products $(S^z)^{2S+1-m}(S^+)^m$, Eq.(7) has to be multiplied *from the left* by $(S^z)^l$. Eqs.(8) – (10) remain unchanged if $S^-S^+(S^z)^i$ is substituted by $(S^z)^iS^-S^+$, since S^-S^+ is diagonal in the S^z representation. Thus the products $(S^z)^{2S+1-m}(S^+)^m$ are replaced by

$$(S^z)^{2S+1-m}(S^+)^m = \sum_{i=0}^{2S-m} \delta_i^{(S,m)} (S^z)^i (S^+)^m. \quad (13)$$

7) The corresponding reduction of spin operator products with an arbitrary order of the operators S^+ , S^- , and S^z , for example $(S^z)^{2S+1-m}(S^-)^m$, can be deduced from Eqs.(12),(13) by the usual commutation relations of the spin operators. Products consisting both S^+ and S^- may be facilitated with the help of Eq.(7). If the total power is larger than $2S + 1$, at first a particular subset of spin operators can be reduced. Then by repeated application of the procedure the complete spin operator product is replaced by a sum of products with a maximal total power equal to $2S$.

8) At the end of this derivation we like to remark a few important points.

(i) The described procedure for the reduction of the local spin operator products is *exact*, no approximation has been used. Products of spin operators located on different lattice sites, for example due to the exchange interaction, cannot be considered by the procedure outlined here.

(ii) The above results are valid for a sum of powers equal to or larger than $2S + 1$. The operators $(S^\pm)^m$ in Eqs.(12),(13) must not be cancelled, since this will lead to wrong results. For instance, cancellation of the common factor $(S^-)^m$ in Eq.(12) leads to the relation between powers of S^z given by $(S^z)^{2S+1-m} = \sum_{i=0}^{2S-m} \delta_i^{(S,m)} (S^z)^i$. However, this relation is *only* correct for $m = 0$, i.e. Eq.(3) !

- (iii) Facilitating the powers $(S^z)^{l+1}$ by replacing the products S^-S^+ on the right hand side of Eq.(8) – (10) with the help of Eq.(3) does not help since this leads to identities.
- (iv) Similar as for the coefficients α in Eq.(3) there should exist also recursion relations for the coefficients β , γ , and δ of Eqs.(8) – (13), connecting respective coefficients for different spin quantum numbers S . We have not taken here the effort to deduce them.

In conclusion, in this study we have shown how the total power of arbitrary products of spin operators $(S^+)^l(S^-)^m(S^z)^n$ can be reduced by one unit, if the sum of its powers is equal to $2S + 1$. In addition we emphasize that by a repeated application of the procedure *all* arbitrary spin operator products with a total power larger than $2S + 1$ can be replaced by a sum of spin operators with a maximum total power of $2S$. These transformations are exact. It is important to note that the procedure outlined here is valid for *local* spin operator products only, i.e. all involved spin operators belong to the same lattice site. For example, the magnetic anisotropies, determining the direction of the magnetization, are usually single-ion quantities. We note that the consideration of such a single-ion anisotropy of l -th order are only supported by spin quantum numbers $2S \geq l$ [10,12,20,21]. Vice versa, for a given S the maximum order of distinct anisotropy terms as considered in the Heisenberg Hamiltonian is limited since anisotropy orders larger than $2S$ can be replaced by lower order ones. This is due to exactly the same circumstances leading to the reduction of spin operator products outlined here. Note also that single-ion anisotropy terms can be replaced by irreducible tensor operators [10,12,20,21]. Furthermore, the investigation of the magnetic properties within a Green’s function theory can be facilitated [14–17]. For instance, the higher order Green’s functions appearing in the equation of motion can be replaced by lower order ones without approximation, if the involved *local* spin operators are reduced along the lines described here.

Localized, quantum mechanical spins are present in the strongly correlated rare earth magnets, in which the localized $4f$ - electrons cause the magnetic state. On the other hand, the $3d$ - magnets are itinerant electron systems, the electrons causing the magnetism are not as localized as in the $4f$ - systems, and the quantum mechanical nature of the *equilibrium*

state of the magnetic properties may be hidden. This can be seen for example from the arbitrary values of the resulting magnetic moments. Consequently, its magnetic properties are usually represented by three-dimensional *classical* spin vectors $S \rightarrow \infty$. However, the quantum mechanical nature of the magnetism of these band magnets should be visible in the ultrashort time domain, for example within the magnetic relaxation after an excitation [22]. Such ultrashort temporal properties in the fsec- time domain can nowadays be investigated experimentally [23,24]. For the theoretical study of these time dependent magnetic properties, which can be accomplished e.g. by application of a *time dependent* Green's function (Keldysh-) formalism [25], the reduction of the spin operator products may be a very useful tool.

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	$m = 0$						$m = 1$					$m = 2$				$m = 3$			$m = 4$	$m = 5$		
S	$\delta_0^{(S,0)}$	$\delta_1^{(S,0)}$	$\delta_2^{(S,0)}$	$\delta_3^{(S,0)}$	$\delta_4^{(S,0)}$	$\delta_5^{(S,0)}$	$\delta_0^{(S,1)}$	$\delta_1^{(S,1)}$	$\delta_2^{(S,1)}$	$\delta_3^{(S,1)}$	$\delta_4^{(S,1)}$	$\delta_0^{(S,2)}$	$\delta_1^{(S,2)}$	$\delta_2^{(S,2)}$	$\delta_3^{(S,2)}$	$\delta_0^{(S,3)}$	$\delta_1^{(S,3)}$	$\delta_2^{(S,3)}$	$\delta_0^{(S,4)}$	$\delta_1^{(S,4)}$	$\delta_0^{(S,5)}$	
$\frac{1}{2}$	$\frac{1}{4}$	0	-	-	-	-	$\frac{1}{2}$	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
1	0	1	0	-	-	-	0	1	-	-	-	1	-	-	-	-	-	-	-	-	-	-
$\frac{3}{2}$	$-\frac{9}{16}$	0	$\frac{10}{4}$	0	-	-	$-\frac{3}{8}$	$\frac{1}{4}$	$\frac{3}{2}$	-	-	$-\frac{3}{4}$	2	-	-	$\frac{3}{2}$	-	-	-	-	-	-
2	0	-4	0	5	0	-	0	-2	1	2	-	0	-2	3	-	-2	3	-	2	-	-	-
$\frac{5}{2}$	$\frac{225}{64}$	0	$-\frac{259}{16}$	0	$\frac{35}{4}$	0	$\frac{45}{32}$	$-\frac{9}{16}$	$-\frac{25}{4}$	$\frac{5}{2}$	$\frac{5}{2}$	$\frac{15}{16}$	-1	$-\frac{7}{2}$	4	$\frac{15}{8}$	$-\frac{23}{4}$	$\frac{9}{2}$	$-\frac{15}{4}$	4	$\frac{5}{2}$	

Table 1: Coefficients $\delta_i^{(S,m)}$ occurring in Eqs.(12),(13) for several values of the spin quantum number $S = 1/2, 1, 3/2, 2, 5/2$.